structure search

Connecting via Winsock to STN

10/629,858

Welcome to STN International! Enter x:
x
Welcome to STN International! Enter x:
LOGINID:sssptau121bd

PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 14:29:28 ON 29 SEP 2004
FILE 'REGISTRY' ENTERED AT 14:29:28 ON 29 SEP 2004

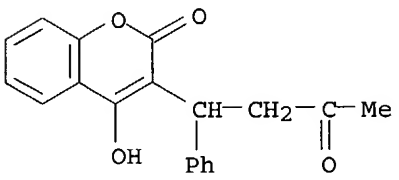
=> s warfrin/cn
L2 0 WARFRIN/CN

=> s warfarin/cn
L3 1 WARFARIN/CN

=> d ide

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 81-81-2 REGISTRY
CN 2H-1-Benzopyran-2-one, 4-hydroxy-3-(3-oxo-1-phenylbutyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Coumarin, 3-(α-acetonylbenzyl)-4-hydroxy- (7CI, 8CI)
OTHER NAMES:
CN (±)-Warfarin
CN (±)-Warfarin-alcohol
CN (RS)-Warfarin
CN 1-(4'-Hydroxy-3'-coumarinyl)-1-phenyl-3-butanone
CN 3-(α-Acetonylbenzyl)-4-hydroxycoumarin
CN 3-(α-Phenyl-β-acetylethyl)-4-hydroxycoumarin
CN 3-(1'-Phenyl-2'-acetylethyl)-4-hydroxycoumarin
CN 4-Hydroxy-3-(3-oxo-1-phenylbutyl)-2H-chromen-2-one
CN Athrombine-K
CN Brumolin
CN Co-Rax
CN Compound 42
CN Coumafen
CN Coumafene
CN Coumaphen
CN Coumefene
CN Dethmor
CN DL-3-(α-Acetonylbenzyl)-4-hydroxycoumarin
CN Kumader
CN Kumadu
CN Kumatox
CN NSC 59813
CN rac-Warfarin
CN Ratron
CN Ratron G
CN Rodafarin
CN Rodafarin C
CN Rodex
CN Temus W
CN Vampirinip II
CN Vampirinip III
CN W.A.R.F. 42

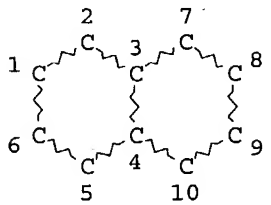
CN WARF compound 42
CN **Warfarin**
CN Zoocoumarin
FS 3D CONCORD
DR 56573-89-8, 5543-56-6
MF C19 H16 O4
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DIOGENES, EMBASE, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IMSCOSEARCH, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PIRA, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, ULIDAT, USAN, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PREP (Preparation); PRP (Properties); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

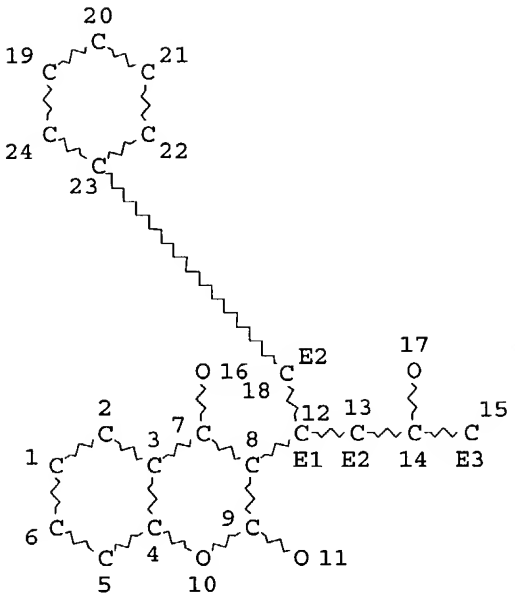
3490 REFERENCES IN FILE CA (1907 TO DATE)
49 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
3507 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> str
:gra r66,dis



:=> d sia
L4 HAS NO ANSWERS

L4 STR



NODE ATTRIBUTES:
HCOUNT IS E1 AT 12
HCOUNT IS E2 AT 13
HCOUNT IS E3 AT 15
HCOUNT IS E2 AT 18
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

=> s l4
SAMPLE SEARCH INITIATED 14:36:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 5 TO 234
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s l4 ful
FULL SEARCH INITIATED 14:37:02 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 75 TO ITERATE

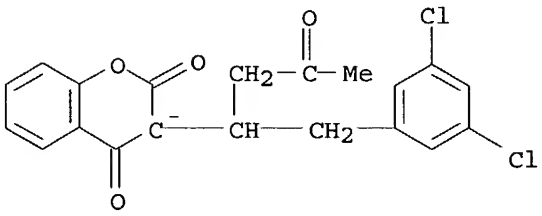
100.0% PROCESSED 75 ITERATIONS 13 ANSWERS
SEARCH TIME: 00.00.01

L6 13 SEA SSS FUL L4

=> d scan

L6 13 ANSWERS REGISTRY

IN 2H-1-Benzopyran-2,4(3H)-one, 3-[1-[(3,5-dichlorophenyl)methyl]-3-oxobutyl]-, ion(1-), sodium (9CI)
MF C20 H15 Cl2 O4 . Na



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

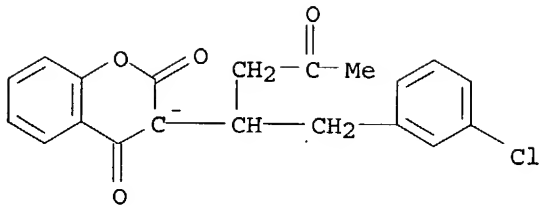
=> d reg can tot

1	RN	749207-45-2	REGISTRY
2	RN	734532-29-7	REGISTRY
3	RN	732244-73-4	REGISTRY
4	RN	723242-03-3	REGISTRY
5	RN	673472-73-6	REGISTRY
REFERENCE 1: 140:264500			
6	RN	673472-71-4	REGISTRY
REFERENCE 1: 140:264500			
7	RN	673472-69-0	REGISTRY
REFERENCE 1: 140:264500			
8	RN	673472-67-8	REGISTRY
REFERENCE 1: 140:264500			
9	RN	673472-65-6	REGISTRY
REFERENCE 1: 140:264500			
10	RN	673472-63-4	REGISTRY
REFERENCE 1: 140:264500			
11	RN	673472-61-2	REGISTRY
REFERENCE 1: 140:264500			
12	RN	673472-59-8	REGISTRY
REFERENCE 1: 140:264500			
13	RN	673472-57-6	REGISTRY
REFERENCE 1: 140:264500			

=> d 1 sub bib abs

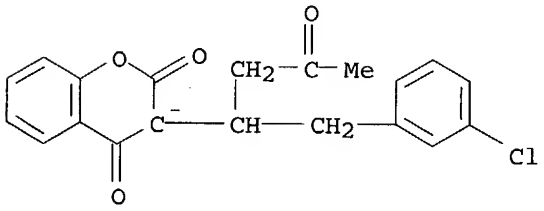
L6 ANSWER 1 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN 749207-45-2 REGISTRY
CN 2H-1-Benzopyran-2,4(3H)-one, 3-[1-[(3-chlorophenyl)methyl]-3-oxobutyl]-, ion(1-) (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H16 Cl O4
CI COM

SR CA



=> d 1

L6 ANSWER 1 OF 13 REGISTRY COPYRIGHT 2004 ACS on STN
RN 749207-45-2 REGISTRY
IN 2H-1-Benzopyran-2,4(3H)-one, 3-[1-[(3-chlorophenyl)methyl]-3-oxobutyl]-, ion(1-) (9CI)
MF C20 H16 Cl O4



=> fil beil
FILE 'BEILSTEIN' ENTERED AT 14:39:02 ON 29 SEP 2004
COPYRIGHT (c) 2004 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON JUNE 15, 2004

FILE COVERS 1771 TO 2003.
*** FILE CONTAINS 8,997,153 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

****
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *

```
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE  *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE         *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                       *
* FOR PRICE INFORMATION SEE HELP COST                               *
*********************************************************************
    NEW
* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE
  SEARCHED, SELECTED AND TRANSFERRED.
* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES,
  ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A
  COMPOUND AT A GLANCE.

*** YOU HAVE NEW MAIL ***

=> d his

     (FILE 'HOME' ENTERED AT 13:34:19 ON 29 SEP 2004)

     FILE 'REGISTRY' ENTERED AT 13:34:30 ON 29 SEP 2004
L1             1 S LAETISPICINE/CN
L2             0 S WARFRIN/CN
L3             1 S WARFARIN/CN
L4               STR
L5             0 S L4
L6            13 S L4 FUL

     FILE 'BEILSTEIN' ENTERED AT 14:39:02 ON 29 SEP 2004

=> s l4 ful
FULL SEARCH INITIATED 14:39:17 FILE 'BEILSTEIN'
FULL SCREEN SEARCH COMPLETED -      11 TO ITERATE

100.0% PROCESSED      11 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.04

L7             0 SEA SSS FUL L4

=> fil caplus
FILE 'CAPLUS' ENTERED AT 14:39:28 ON 29 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 29 Sep 2004  VOL 141 ISS 14
FILE LAST UPDATED: 28 Sep 2004  (20040928/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l6
L8             1 L6

=> d cbib abs
```

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

2004:252198 Document No. 140:264500 Safer anticoagulant effect of coumarin analog compounds. Carter, Daniel C. (USA). U.S. Pat. Appl. Publ. US 2004058985 A1 20040325, 13 pp. (English). CODEN: USXXCO. APPLICATION: US 2003-629858 20030730. PRIORITY: US 2002-PV399126 20020730.

AB The invention discloses the albumin-guided development of coumarin analogs which can be used as safer and more effective alternatives to previous analogs such as sodium warfarin. The coumarin analogs of the invention are identified and isolated by the fact that they have binding sites to albumin which are different than the binding sites of conventional coumarin analogs such as sodium warfarin, and as a result will be less prone to be displaced since the binding site of sodium warfarin is shared by numerous drugs such as aspirin. The invention also discloses methods of providing anticoagulant and antithrombotic treatment utilizing effective amts. of the coumarin analogs which will have reduced potential for unfavorable drug interactions, reduced metabolic complications, and improved controllability within their therapeutic range. Together, the coumarin analogs of the invention are advantageous because they can achieve the effects of the prior coumarin analogs with a min. of metabolic complications and undesirable side effects.

=> log h

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	3.43	196.70

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.70	-1.36

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 14:40:33 ON 29 SEP 2004

```
=> d his

     (FILE 'HOME' ENTERED AT 09:23:12 ON 30 SEP 2004)

     FILE 'REGISTRY' ENTERED AT 09:23:22 ON 30 SEP 2004
L1                STR
L2              0 S L1
L3                STR L1
L4              0 S L3
L5                STR L3
L6              0 S L5
L7              3 S L5 FUL

     FILE 'CAPLUS' ENTERED AT 09:34:21 ON 30 SEP 2004
L8              1 S L7

=> d sia l5
L5 HAS NO ANSWERS
L5                STR
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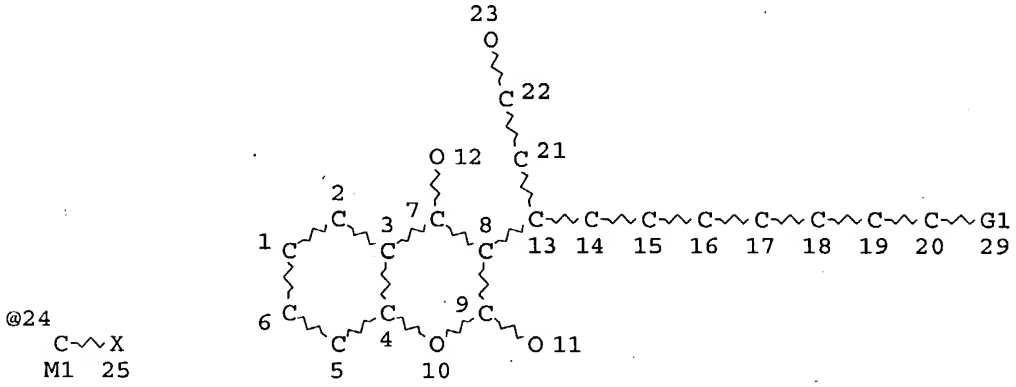

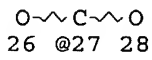


```
VAR G1=24/27/ME/ET/N-PR/I-PR
NODE ATTRIBUTES:
HCOUNT  IS M1     AT  24
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  29

STEREO ATTRIBUTES: NONE
```